Diethyl sulfate

64-67-5 | DTXSID1024045

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -14.8 °C

Global applicability domain: Inside

Local applicability domain index: 5.69e-01

Confidence level: 4.29e-01

Nearest Neighbors from the Training Set

Image not found
Diethyl sulfate
Measured: -24.0
Predicted: -14.8

Image not found
Dimethyl sulfate
Measured: -27.0
Predicted: -17.2

Image not found
Propanedioic acid, oxo-, diethyl ester
Measured: -30.0
Predicted: 1.01e-01

Image not found
Ethylene glycol, cyclic sulfate
Measured: 99.0
Predicted: 56.4

Image not found
Ethyl 2,4-dioxovalerate
Measured: 18.0
Predicted: 27.4